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N-Heterocyclic Carbene Adducts of Molybdenum tetra-Carboxylate Complexes.

Thomas P. Robinson,[a] Andrew L. Johnson,[a]* Paul R. Raithby,[a] and Gabriele Kociok-Kohn.[b]

[a] *Department of Chemistry, University of Bath, Claverton Down, Bath, BA2 7AY, UK.* [b] *Chemical Crystallography Unit, Department of Chemistry, University of Bath, Claverton Down, Bath, BA2 7AY, UK.*Email:

A.L.Johnson@bath.ac.uk

Table 1S: X-ray Crystallographic Data for Compounds **1a**, **2a**, **3a** and **1b**.

	(**1a**)	(**2a**)	(**3a**)	(**1b**)
Empirical Formula	$C_{29}H_{24}F_{12}Mo_2N_2O_8$	$C_{29}H_{36}Mo_2N_2O_8$	$C_{44.50}H_{64}Mo_2N_2O_8$	$C_{70}H_{82}F_{12}Mo_2N_4O_8$
FW ($g.mol^{-1}$)	948.38	732.48	946.85	1527.27
Crystal System	Monoclinic	Triclinic	Monoclinic	Orthorhombic
Space Group	$P2_1/n$	P-1	$P2_1/a$	$P2_12_12_1$
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
a (Å)	8.5050(2)	8.4000(2)	11.2778(2)	16.61270(10)
b (Å)	17.1100(3)	17.3732(4)	27.5134(6)	19.3204(2)
c (Å)	24.4660(3)	21.3704(4)	15.7145(4)	45.9155(5)
α (°)	90	84.852(2)	90	90
β (°)	95.5790(10)	87.660(2)	97.019(2)	90
γ (°)	90	76.240(2)	90	90
Volume ($Å^3$)	3543.44(11)	3016.35(12)	4839.52(18)	14737.2(2)
Crystal Size (mm^3)	0.200 x 0.150 x 0.150	0.250 x 0.250 x 0.200	0.770 x 0.230 x 0.120	0.300 x 0.250 x 0.250
Density (Mgm^{-3})	1.778	1.613	1.300	1.377
Z	4	4	4	8
μ (Mo Kα) (mm^{-1})	0.820	0.883	0.566	0.424
Theta range (°)	7.876 to 27.494	3.021 to 29.440	2.791 to 27.500	3.550 to 25.009
Reflections Collected	55010	22264	52926	163154
Independent Reflections	7882	13796	11088	25323
R_{int}	0.0675	0.0311	0.0264	0.1260
R_1 .wR_2 $[I>2\sigma(I)]$	0.0347, 0.0684	0.0421, 0.0711	0.0323, 0.0812	0.0706, wR2 = 0.1079
R indices (all data)	0.0561, 0.0754	0.0746, 0.0823	0.0392, 0.0855	0.1138, wR2 = 0.1177
Flack Parameter	-	-	-	0.126(14)
Largest diff. peak and hole ($e.Å^{-3}$)	0.739, -0.505	0.867, -0.555	1.132, -0.565	0.590, -0.500
CCDC Reference	1477588	1477587	1477589	1477590

Table 2S: X-ray Crystallographic Data for Compounds **1c**, **1d**, **2d**, **4** and **5**.

	(1c)	(1d)	(2d)	(4)	(5)
Empirical Formula	$C_{26}H_{32}F_{12}Mo_2N_4O_8$	$C_{30}H_{40}F_{12}Mo_2N_4O_8$	$C_{58}H_{84}Mo_2N_4O_8$	$C_{36}H_{66}Mo_2N_2O_{10}$	$C_{40}H_{62}Cl_2Mo_2N_4O_4$
FW ($g.mol^{-1}$)	948.43	1004.54	1157.17	878.78	925.71
Crystal System	Triclinic	Monoclinic	Triclinic	Monoclinic	Triclinic
Space Group	*P*-1	$P2_1/n$	*P*-1	Cc	*P*-1
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
a (Å)	11.3739(6)	9.8400(2)	8.5480(2)	12.21900(10)	9.8940(2)
b (Å)	12.0093(7)	12.2550(3)	11.9010(3)	21.1750(2)	11.8630(2)
c (Å)	13.5043(8)	16.1040(2)	15.0010(4)	17.9860(2)	12.7570(3)
α (°)	90.405(5)	90	100.6310(10)	90	102.557(1)
β (°)	106.754(5)	91.3730(10)	102.629(2)	103.5920(10)	106.210(1)
γ (°)	91.534(4)	90	102.0870(10)	90	93.427(1)
Volume ($Å^3$)	1765.44(18)	1941.41(7)	1413.08(6)	4523.32(8)	1391.76(5)
Crystal Size (mm^3)	0.200 x 0.100 x 0.100	0.500 x 0.380 x 0.380	0.300 x 0.130 x 0.080	0.200 x 0.100 x 0.050	0.200 x 0.130 x 0.100
Density (Mgm^{-3})	1.784	1.718	1.360	1.290	1.214
Z	2	2	1	4	1
μ (Mo Kα) (mm^{-1})	0.824	0.755	0.499	0.603	0.585
Theta range (°)	3.167 to 28.279	7.929 to 31.017	8.516 to 27.421	4.142 to 32.004	3.544 to 30.687
Reflections Collected	15978	30529	26722	50052	8488[a] ()
Independent Reflections	8722	6069	6165	14898	8488
R_{int}	0.0314	0.0298	0.0688	0.0692	0.0373[b]
R_1 .wR_2 [I>2σ(I)]	0.0492, 0.1138	0.0321, 0.0810	0.0300, 0.0690	0.0351, 0.0853	0.0355, 0.1174
R indices (all data)	0.0674, 0.1269	0.0363, 0.0838	0.0386, 0.0728	0.0440, 0.0929	0.0412, 0.1212
Flack Parameter	-	-	-	0.17(3)	-
Largest diff. peak and hole	1.892, -1.069	1.213, -1.259	0.602, -0.654	0.702, -0.642	1.83, -0.75
CCDC Reference	1477591	1477593	1477592	1477594	1477595

[a] after SQUEEZE;[b] before SQUEEZE

S1: Molecular structure of complex 2d

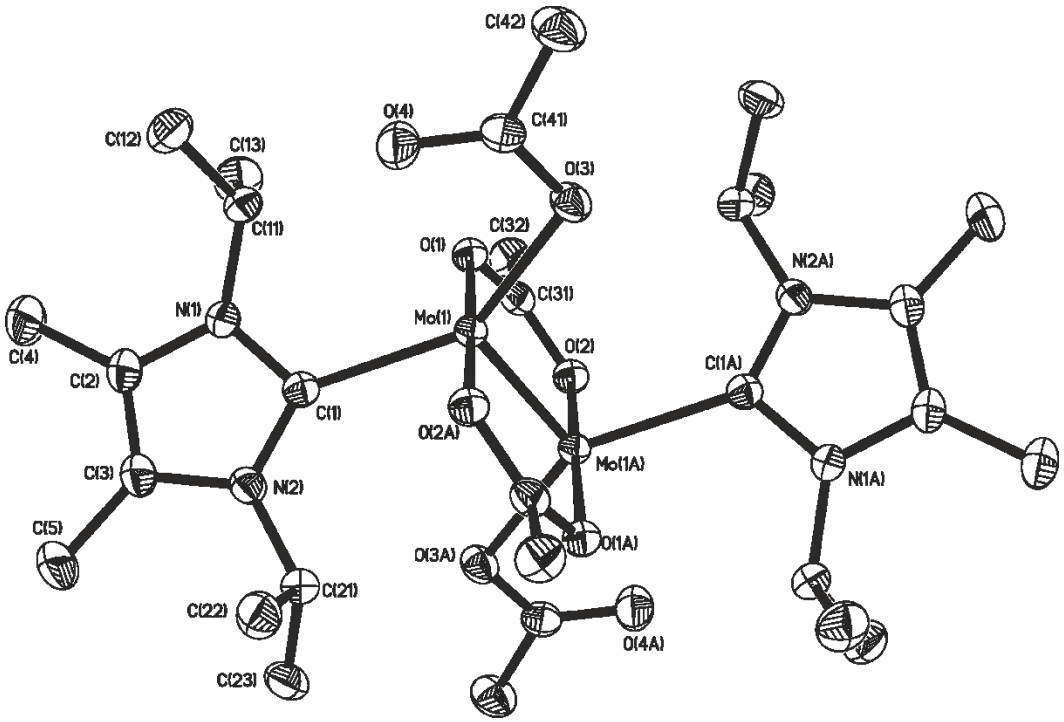

Figure S1: Molecular structure of the molecular structure $[Mo_2(\mu\text{-}OAc)_2(OAc)_2(\mathbf{L^d})_2]$ (**2d**). The solvent of crystallisation and hydrogen atoms have been removed for clarity, and thermal ellipsoids are shown at 50 % probability. Symmetry transformations used to generate equivalent atoms: 1 -x,-y,-z+1.